

Patent claims

1. Compound of the general formula (I)

$$X(B)_m \quad (I)$$

wherein

X is an m-valent unit and

B are identical or different and denote K-R,

wherein

K is a bond or is $A^1-(A^2-A^3)_k-sp$, wherein A^1 is $(CH_2)_tY(CH_2)_u$, whereinY is $>C=O$, $>NH$, $-O-$, $-S-$ or a bond,

t is an integer from 0 to 6 and

u is an integer from 0 to 6,

 A^2 is $-NHCO-$, $-CONH-$, $-OCONH-$ or $SCONH-$, or is $-CO-$, A^3 is $(CH_2)_r$, $O(CH_2)_r$, $NH(CH_2)_r$, $S(CH_2)_r$ or $-(CHQ)-$, wherein

r is an integer from 1 to 6 and

Q is a substituted or unsubstituted alkyl or aryl group,

sp is a divalent spacer or a bond, and

k is an integer from 5 to 100, and

R is hydrogen; a ligand suitable for specific bonding to a receptor; a marker molecule; or a catalytically active group; and

m is at least 2,

with the proviso that

- (1) in the compound at least one R is not hydrogen,
- (2) there are at least two K that are not a bond, and
- (3) X, B and m are so selected that an intermolecular association of the K in liquid phase by the formation of hydrogen bonds is possible, with formation of aggregates that present on the surface a plurality of R that are not hydrogen, and
- (4) the molar mass of the fragment $X(K)_m$ is less than 20,000.

2. Compound according to claim 1, wherein the molar mass of the fragment $X(K)_m$ is less than 4,000.

3. Compound according to either claim 1 or claim 2, wherein

m is an integer from 2 to 4, and
X is CH_{4-m} , NH_{3-m} , N^+H_{4-m} , $>\text{P}-$ (when m = 3), $>\text{P}^+<$ (when m = 4), $>\text{B}-$ (when m = 3), a linear atom group C_2H_{6-m} , $>\text{CH}(\text{CH}_2)_z\text{CH}<$, $>\text{C}=\text{C}<$, $>\text{N}-\text{N}<$, $>\text{N}(\text{CH}_2)_z\text{N}<$ wherein z = 2 - 6, when m = 4), a carbocyclic atom group C_6H_{6-m} , $\text{C}_6\text{H}_{12-m}$, or a heterocyclic atom group C_3N_3 (when m = 3), C_4N_2 (when m = 4).

4. Compound according to any one of claims 1 to 3, wherein there are at least 3 K.
5. Compound according to any one of claims 1 to 4, wherein at least two R are not hydrogen.
6. Compound according to any one of claims 1 to 4, wherein at least three R are not hydrogen.
7. Compound according to any one of claims 1 to 6, wherein the ligand R is a mono- or oligo-saccharide, a peptide, a mono- or oligo-nucleotide or a nucleic base and their derivatives and mimetics.
8. Compound according to claim 7, wherein the saccharide R is sialic acid, sialyl lactose, sialyl lactosamine, lactose, mannose, $\text{Gal}\alpha 1-3\text{Gal}$, $\text{Gal}\alpha 1-3(\text{Fuc}\alpha 1-2)\text{Gal}$, $\text{GalNAc}\alpha 1-3(\text{Fuc}\alpha 1-2)\text{Gal}$, Neu5Aca2-6GalNAc , SiaLe^A , SiaLe^X , HSO_3Le^A , HSO_3Le^X , $\text{Gal}\alpha 1-3\text{Gal}\beta 1-4\text{GlcNAc}$, $\text{Gal}\alpha 1-3\text{Gal}\beta 1-4\text{Glc}$, $\text{HSO}_3\text{GlcA}\beta 1-3\text{Gal}\beta 1-4\text{GlcNAc}$, N-acetyl-lactosamine or polylactosamine, or wherein the saccharide is sialic acid benzyl glycoside, $\text{HSO}_3\text{GlcA}\beta 1-3\text{Gal}$, $\text{HSO}_3\text{GlcA}\beta 1-3\text{Gal}\beta 1-4\text{GlcNAc}\beta 1-3\text{Gal}\beta 1-4\text{Glc}$, $\text{GalNAc}\alpha$, $\text{GalNAc}\alpha 1-3(\text{Fuc}\alpha 1-2)\text{Gal}\beta 1-4\text{GlcNAc}$, $\text{Gal}\alpha 1-3(\text{Fuc}\alpha 1-2)\text{Gal}\beta 1-4\text{GlcNAc}$, $\text{HSO}_3(\text{Sia})\text{Le}^X$, $\text{HSO}_3(\text{Sia})\text{Le}^A$, Le^Y , $\text{GlcNAc}\beta 1-6(\text{GlcNAc}\beta 1-3)\text{Gal}\beta 1-4\text{Glc}$, $\text{GalNAc}\beta 1-4(\text{Neu5Aca2-3})\text{Gal}\beta 1-4\text{Glc}$, mannose-6-phosphate, $\text{GalNAc}\beta 1-4\text{GlcNAc}$, oligo-sialic acid, N-glycolylneuraminic acid, $\text{Gal}\alpha 1-4\text{Gal}\beta 1-4\text{Glc}$, $\text{Gal}\alpha 1-4\text{Gal}\beta 1-4\text{GlcNAc}$.
9. Compound according to any one of claims 1 to 8, wherein
 - m is an integer from 2 to 4,
 - X is CH_{4-m} ,
 - A^1 is CH_2 ,
 - A^2 is NHCO ,
 - A^3 is CH_2 ,
 - k is 8,
 - sp is $(\text{CH}_2)_3\text{CONHCH}_2\text{CONHC}_6\text{H}_4-4-\text{CH}_2\text{O}-$ and

R is Neu5Ac α 2-6Gal β 1-4GlcNAc.

10. Aggregate of the general formula (II):

{X(B)_m}_n (II)

wherein

X(B)_m may be identical or different and denote a compound of the general formula (I), as defined in any one of claims 1 to 11, and

n is from 2 to 100,000,

and wherein X(B)_m are non-covalently bonded.

11. Aggregate according to claim 10 having a leaf-like, linear, cyclic, polycyclic, polyhedral, spherical or dendritic structure.

12. Aggregate according to claim 10 or 11 of two or more different compounds according to any one of claims 1 to 9.

13. Process for the preparation of an aggregate as defined in any one of claims 10 to 12 by self-association of compounds according to any one of claims 1 to 9.

14. Process according to claim 13, comprising in the case of a solution of the compound addition of a concentrated salt solution, a change in the pH or the temperature or addition of organic solvents.

15. Process for changing the structure of the aggregate as defined in any one of claims 10 to 12, which comprises addition of a concentrated salt solution, a change in the temperature or the pH or an addition of urea, trifluoroethanol or peptides.

16. Process for increasing the specific physiological activities of molecules by their incorporation as radical R into a compound of the general formula (I) as defined in any one of claims 1 to 9 or into an aggregate of the general formula (II) as defined in any one of claims 10 to 12.

17. Preparation, comprising a compound as defined in any one of claims 1 to 9 or an aggregate as defined in any one of claims 10 to 12, for use in therapeutic or diagnostic procedures.

18. Preparation according to claim 17 against inflammation, viral and bacterial infections, influenza viruses, selectin-mediated inflammatory processes, tumour metastases, or in the neutralisation of antibodies in autoimmune disorders and transplants.

19. Use of a compound as defined in any one of claims 1 to 9 or of an aggregate as defined in any one of claims 10 to 12 in the preparation of a medicament against inflammation, viral and bacterial infections, influenza viruses, selectin-mediated inflammatory processes, tumour metastases, or in the neutralisation of antibodies in autoimmune disorders and transplants.

20. Use of a compound as defined in any one of claims 1 to 9 or of an aggregate as defined in any one of claims 10 to 12 in the preparation of functionalised molecular surfaces.

21. Use of a compound as defined in any one of claims 1 to 9 or of an aggregate as defined in any one of claims 10 to 12 in an analytical procedure.

22. Use according to claim 21 in a diagnostic procedure.

23. Compound of the general formula (III),

$X(B)_m$ (III)

wherein

X is an m -valent unit and

B are identical or different and denote K-H,

wherein

K is $A^1-(A^2-A^3)_k-sp$,

wherein

A^1 is $(CH_2)_tY(CH_2)_u$, wherein

Y is $>C=O$, $>NH$, $-O-$, $-S-$ or a bond,

t is an integer from 0 to 6 and

u is an integer from 0 to 6,

A^2 is $-NHCO-$, $-CONH-$, $-OCONH-$ or $SCONH-$, or is $-CO-$,

A^3 is $(CH_2)_r$, $O(CH_2)_r$, $NH(CH_2)_r$, $S(CH_2)_r$ or $-(CHQ)-$, wherein

r is an integer from 1 to 6 and

Q is a substituted or unsubstituted alkyl or aryl group,

sp is a divalent spacer or a bond, and
k is an integer from 5 to 100, and

m is at least 2,

with the proviso that

- (1) X, B and m are so selected that an intermolecular association of the K in liquid phase is possible, especially under aqueous conditions, by the formation of hydrogen bonds, with formation of aggregates, and
- (2) the molar mass of the fragment $X(K)_m$ is less than 20,000, especially less than 4000.

24. Use of a compound of the general formula (III) according to either one of claims 22 and 23 in the modification of an aggregate as defined in either one of claims 10 and 11.

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